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Ensemble initial conditions through 4D-Var assimilation

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[1] The methodology to generate members of an ensemble is an important issue in operational forecasting; currently a number of procedures are followed at different operational centres. In the present work we propose and evaluate a methodology where a dynamically consistent set of initial conditions is generated through 4D-Var assimilation procedure. The perturbations are generated through 4D-Var assimilation with different information (observation) content, either through a variation in the frequency of observations or a variation in the length of assimilation window. We adopt a representative non-linear system, viz. the three-variable Lorenz system and show that ensemble forecasts generated through 4D-Var assimilation show less error than those generated from initial conditions (with similar amplitude of perturbation) adopted arbitrarily. Another advantage of the procedure is that it provides a (variable-specific) estimate of the maximum allowed amplitude and spread of perturbations.
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1. Introduction

[2] Ensemble forecasting has emerged as an indispensable tool in meteorological forecasting since its introduction in the early nineties [*Molteni and Palmer*, 1993; *Buizza*, 1997; *Toth and Kalnay*, 1997]. The basic philosophy of ensemble forecasting is to generate a set of forecasts, such that the average of the ensemble of the forecasts is more accurate than a single deterministic forecast. Besides, the spread in the ensemble contains quantitative information about the reliability of forecasts, and provides a basis for probabilistic forecast. An ensemble forecasting, however, should be able to (non linearly) filter errors for it to be considered good, or useful for forecasting. A critical issue in ensemble forecasting is thus how to create a good ensemble, that is, how to create a set of initial perturbations that would result in a better forecast.

[3] A number of techniques and methodologies have evolved since early nineties to generate perturbations for creating an ensemble. One method is to use singular vectors, the linear perturbations of a control forecast that grow fastest within a certain time interval called the optimization period [*Lorenz*, 1965], for a given norm to measure their size. An ensemble forecasting based on initial perturbations based on singular vectors with a total energy norm was operationalised at ECMWF [*Molteni and Palmer*, 1993; *Molteni et al.*, 1996; *Buizza*, 1997; *Palmer et al.*, 1998].The Bred vector method, on the other hand, uses a non-linear generalization of the method to obtain the sustained fastest growing perturbations (Leading Lyapunov vectors [*Toth and Kalnay*, 1993, 1997]). The bred vectors represent forecast perturbations and unlike singular vectors they are independent of the norm. The bred vector method has been implemented at NCEP in 1992 and later at NCMRWF, India and South African Meteorological Weather Services. Variants of bred vector method have also been used by Japanese Meteorological Agency [*Kyouda and Kusunoki*, 2002]. Another methodology, proposed by *Houtekamer et al.* [1996], uses an ensemble of assimilation systems using perturbed observations. However, the ensemble assimilation system introduces perturbations in the best estimate of the initial condition; as such the individual perturbed forecasts (being different from the best estimate) may have less skill than the control forecast, although the ensemble average can be better than the control forecast. Further the random perturbations of the observations are carried out in conformity with the observational error statistics to ensure that the perturbed analyses are not (statistically) far from the control analysis. The methodology for generating ensemble initial conditions is still evolving and currently different centres use their own procedure.

[4] In this work we propose a methodology to generate a set of initial conditions using Four Dimensional Variational assimilation (hereafter 4D-VAR). Instead of considering perturbations to a best estimate as in an ensemble assimilation system, we generate a number of best estimates by taking advantage of certain features of 4D-VAR assimilation system as discussed below. Similarly, the observations are not perturbed, but the number of observations (information) assimilated is slightly varied to generate different estimates; we shall call this informational perturbation to distinguish it from ordinary (random or systematic) perturbation to the fields themselves. The use of 4D-VAR assimilation to generate the estimates ensures that each member is as close an approximation to an allowed model solution as possible, a property unlikely to be shared by a randomly perturbed estimate. As mentioned, this is possible because of the mathematical structure of 4D-Var assimilation.

[5] 4D-VAR is now an established and powerful tool for assimilation of data in meteorology and oceanography following a number of works which showed its applicability to

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Table 1. Values of Parameters for Different Regimes

Set	Parameters α	β	γ	Dynamical Regime
1	100	27	10.6	chaotic
2	10	23	2.66	non-chaotic
3	28	46.92	4	chaotic
4	16	40	3.66	chaotic
5	10	13.92	2.66	non-chaotic
6	10	24.5	2.66	chaotic
7	10	28	2.66	chaotic

realistic situations [*Ghil and Malanotte-Rizzoli*, 1991; *LeDimet and Talagrand*, 1986; *Talagrand and Courtier*, 1987]. Briefly, 4D-VAR attempts a direct explicit minimization of some scalar function to seek a (non-linear) best estimate of the flow. The scalar function, or the objective function, J, to be minimized is some representation of misfit between the observations X_0 and the model solution; typically, J is the sum of squared differences between observations and the corresponding model solutions X, weighted by the inverse covariance matrix R of the observational errors [*Talagrand*, 1997]. The estimate (or the optimum) value of X, is then the value of X that minimizes J. The gradient of the objective function with respect to the initial condition X(0) for a forecast is given by

$$\nabla_{X(0)} J = \hat{X}(0) \tag{1}$$

where $\hat{X}$ is obtained by integrating the adjoint of the forecast equation (in practice the adjoint code) backward in time; a term involving $(X - X_0)$ appears as a forcing in the adjoint equation. The basic principle of 4D–VAR assimilation is to determine X (t = 0) that will minimize the gradient of the objective function.

[6] Let us consider an objective function of the form

$$J = \frac{1}{N} \sum_{n=1}^{N} |(X(n) - X_0(n))|^2 \tag{2}$$

where N represents the total number of discrete observations.

[7] It is clear that a variation in the amount of information, through a variation in N will change J, which, in turn, will change the estimated state, at least in principle. A typical 4D-VAR assimilation experiment is carried out with a given length of assimilation interval or window (hereafter AI) and a given frequency of observations (hereafter OF). While the later is generally constrained by the observation schedule, the former can be varied relatively easily. A change in either AI or in OF would mean a change in N. We may call such a variation an informational perturbation (with respect to a reference initial state) which will affect the corresponding forecasts; for strongly non-linear systems like the atmosphere and the ocean these effects can be significant. A set of 4D-Var assimilations, with N varied in an optimal range, will thus produce a set of estimates (initial conditions) which are dynamically consistent, with a spread that is also determined in an objective and dynamically consistent manner. We investigate this issue using a representative non-linear system, viz. The Lorenz system with three variables, described by the equations:

$$\begin{aligned} \dot{X}_1 &= \alpha(X_2 - X_1) \\ \dot{X}_2 &= \gamma X_1 - X_2 - X_1 X_3 \\ \dot{X}_3 &= X_1 X_2 - \beta z \end{aligned} \tag{3}$$

Where α, β and γ are real, positive parameters. The Lorenz system is highly representative of the atmospheric and oceanic dynamics in terms of its strong sensitivity to initial conditions. It has also been used to investigate generation of initial conditions [*Anderson*, 1996]. It is well known that this system can represent different dynamical regimes depending on the values of the parameters, especially β. Table 1 gives the seven sets of parameters that were considered in this study.

[8] The 4D-Var assimilation experiments in the present case were designed as follows: First, 'observations' were created by integrating the Lorenz model from a given initial condition. Next, 4D-Var assimilation was carried out for a given AI and OF; the AI was changed in steps of 6 time steps up to a maximum of 120 time steps. Although a longer AI implies more (observational) information incorporated into the assimilation cycle, it also implies a longer integration of the model. The latter may offset gain due to the former due to growth of model error; an optimum AI, therefore, has to be chosen for each assimilation system. The OF was changed between 1–3; for OF = 1 an observation is assimilated every step, while for OF = 3 an observation is assimilated every third time step. The minimization of the objective function was carried out using a variable- storage quasi-Newtonian algorithm [*Gilbert and Lamarèchal*, 1989]. In general terms, the method uses information from the past iterations to approximate the inverse of the Hessian matrix. The inputs to the minimization algorithm are the objective function J, and the gradient of J with respect to the control variable (initial conditions) which must be computed accurately through the adjoint code. This procedure was carried out for a number of dynamical regimes of Lorenz system, represented in terms of α, β and γ, as shown in Table 1. For each dynamical regime, a number of realizations of observations were created by adopting different initial conditions; the five initial conditions used in this study are given in Table 2. In what follows, we shall mostly present results from realization average from these five set of "observations".

Table 2. Set of Initial Conditions

SET	Variables X_1	X_2	X_3
1	8.53	1.95	32.89
2	5	5	35
3	1	0	1
4	−4.5	0.69	23.9
5	2	5	20

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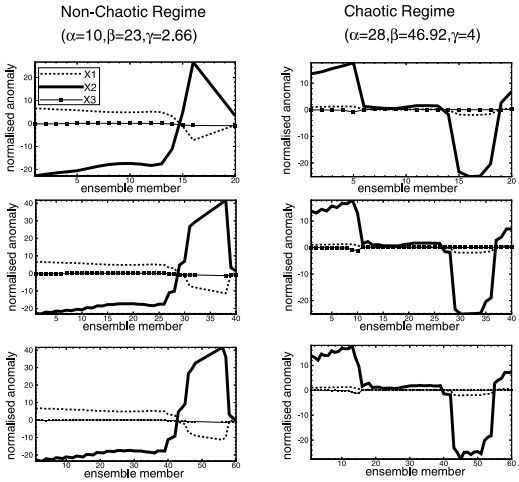

Figure 1. Normalized anomaly (as percentage of ensemble mean) for three variables X_1, X_2 and X_3 of Lorenz equation. The left panel is for a non-chaotic regime while the right panel is for a chaotic regime.

[9] Let $X(i\ ,\ j)$, i = 1,2,3 be the estimate for X_i with the jth 4D-Var assimilation experiment. We can define the ensemble average initial condition as

$$\overline{X}(i) = \frac{1}{N}\sum_{j=1}^{N} X(i,j) \tag{4}$$

Where N is the size of the ensemble.

[10] We can then formally define a perturbation for each i and j as

$$X'(i,j) = X(i,j) - \overline{X}_i \tag{5}$$

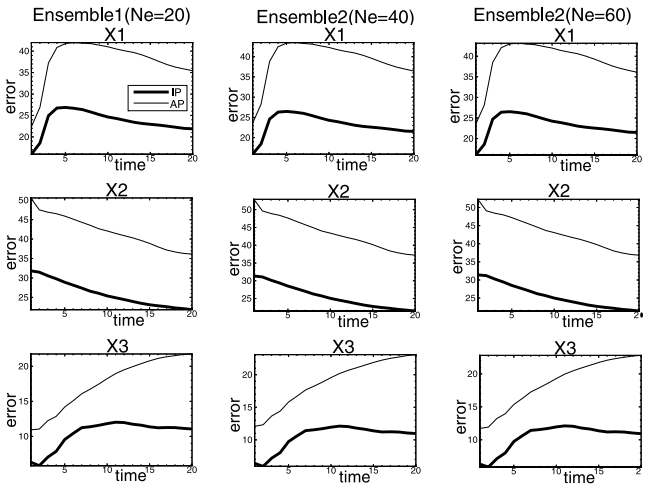

Figure 2. Cumulative growth of forecast error as a function of forecast time (integration step) for the three variables of Lorenz equation for informational perturbation, IP (thick line) and arbitrary perturbation, AP (thin line). The results represent average of five realization of observations for a chaotic regime (α = 100, β = 27, and γ = 10.66).

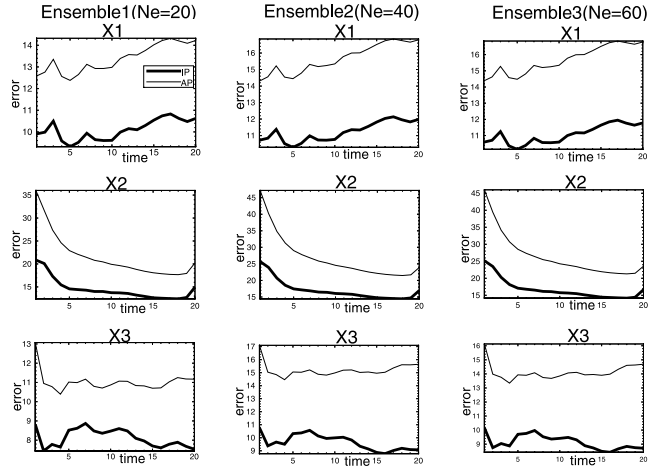

Figure 3. Same as Figure 2 for a non chaotic regime (α = 10, β = 23 and γ = 2.66).

The informationally constructed members of the ensemble can then be formally represented as

$$X_I(i,j) = \overline{X}(i) + X_I'(i,j) \tag{6}$$

In contrast, the non-informationally constructed (arbitrary) members of the ensemble may be represented as

$$X_A(i,j) = \overline{X}(i) + (r)X_I'(i,j) \tag{7}$$

Where r is a random number between -0.8 and 0.8.In constructing the arbitrary perturbations, it is assumed that the knowledge of the ensemble average is available from previous statistical analysis of the system. The amplitude of the random perturbations are constrained to be < = 0.8 to keep X_A (i, j) close to X_I (i, j) in magnitude.

[11] Figure 1 shows the nature of these perturbations in the three variables in terms of percentage of the ensemble mean for different members of the ensemble (x-axis). The spread in X_3 is rather small (a few percents of the ensemble mean) while the spread in $\mathbf{X}_2$ can be as much as 20% or more of the ensemble mean.

[12] We next evaluate relative performance of informational and arbitrary ensemble forecasting in terms of normalized forecast errors, defined as

$$e_{Ai}(j,t) = \frac{1}{N_e}\sum_{j=1}^{N_e} |X_A(i,j)(t) - X_{0i}(t)| \times 100/X_{0i}(t) \tag{8}$$

$$e_{Ii}(j,t) = \frac{1}{N_e}\sum_{j=1}^{N_e} |X_I(i,j)(t) - X_{0i}(t)| \times 100/X_{0i}(t) \tag{9}$$

2. Results and Conclusions

[13] Figure 2 shows the cumulative forecast error, expressed as percentage of the corresponding observation, for three variables of Lorenz system; the thick line

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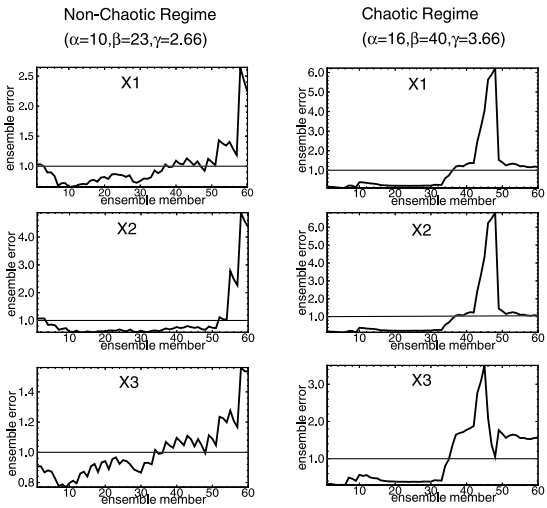

Figure 4. Ratio of time-averaged forecast errors for individual members of the ensemble and ensemble average forecasts for the three variables of the Lorenz system. The left panels represent a non-chaotic regime (α = 10, β = 23 and γ = 2.66) while the right panels represent a chaotic regime (α = 16, β = 40 and γ = 3.66). The X-axis indicates ensemble member.

represents result for informational perturbation (IP) while the thin line shows the corresponding results for arbitrary perturbation (AP). The three columns in Figure 2 represent three ensembles characterized by, respectively, AI = 20, OF = 1; AI = 20, OF = 2 and AI = 20, OF = 3. As mentioned earlier, the results represent average of five realizations of observations obtained by integrating the Lorenz system (for the given regime) with the five initial conditions given in Table 2. It is clear that use of IP can significantly reduces forecast error in comparison to AP.

[14] Figure 3 shows the results corresponding to those in Figure 2 for a non-chaotic regime of Lorenz system, characterized by α = 10, β = 23, and γ = 2.66. Once again initial conditions generated through IP provide about 50% less forecast errors than those generated by AP. It is clear from Figures 2 and 3, however, that the comparative performance also depends on the dynamical regime.

[15] A basic requirement of a successful ensemble forecasting is that the ensemble average forecast is more accurate than forecasts with individual members of the ensemble in general. We examine this aspect for the present methodology in terms of the following quantity:

$$E(j) = \frac{e(j)}{e_e}$$

Where

$$e(j) = \frac{1}{N}\sum_{n=1}^{N} |X(j,n) - X_0(n)|$$

and

$$e_e = \frac{1}{N}\sum_{n=1}^{N} |X_e(n) - X_0(n)|$$

Here X (j, n) is the forecast with initial condition from the jth member of the ensemble and at time step n, and X_e (n) is the ensemble average forecast; X_0 (n) represents the observations.

[16] Figure 4 shows the structure of $E(j)$ for a 60-member ensemble and 20 time steps for two dynamic regimes. It is clear that the ensemble forecast is much more accurate ($E(j) > 1$) than the individual forecasts for a large fraction of the ensemble members. However, for both the dynamical regimes there appears to be a class of members (and hence AI and OF) for which the performance is far superior ($E(j) \gg 1$); these issues need careful reexamination, with other models.

[17] The main purpose of the present work has been to formulate and evaluate a methodology for generating members for an ensemble forecasting through 4D-Var assimilation; the basic premise has been that initial conditions generated through informational perturbations will be dynamically consistent with the total flow in terms of nature of individual members and the spread of the ensemble. This is verified in terms of forecast errors from initial conditions generated through arbitrary perturbations. An important issue is the applicability of the present results with the Lorenz model to multi-scale systems with interacting scales like the atmosphere and the ocean. While the Lorenz model is a good representative of non-linearity and sensitivity of forecast to initial conditions, the ocean and atmosphere have additional complexities such as a wide spectrum of interacting scales and complex boundary forcing. Thus the present conclusions need to be checked with more comprehensive models of atmosphere and ocean. It should also be emphasized that the proposed method is a computationally expensive one for operational numerical weather forecasting as it involves a number of assimilation experiments to generate the IP. However, growing computing power and demand for improved forecast may make such a methodology implementable in near future. Still, a comprehensive and quantitative comparison of skill of the present methodology with methodologies that are relatively cheaper computationally, such as one proposed by *Anderson* [1996] and others, needs to be carried out.

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